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Amphoteric Arsenic in GaN:As

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The >20% lattice mismatch between GaN and GaAs has led to theoretical predictions of strong, composition-dependent band-gap bowing and very limited miscibility of As in GaN [1]. Further predictions that isovalent As could occupy Ga rather than N sites [2], coupled with increasing interest in growing GaNAs alloys for lattice matching with GaP and Si substrates [3], stimulated a structural study of As-doped GaN.

Arsenic *K* near-edge x-ray absorption data from a series of GaN:As samples show that under N-rich MBE growth conditions *As does indeed occupy Ga sites in GaN*. Increasing the Ga flux should lower the formation energy of As in N sites, and this site reversal is also observed. That As can occupy *Ga antisites* and be *amphoteric in GaAs* is not surprising due to the negligible charge exchange between and the similar sizes of Ga and As, but the substantial difference in size between N and As and the large degree of charge transfer between N and Ga makes *amphoteric As in GaN* highly unusual (see figure). The dramatic difference in effective As size when it occupies Ga versus N sites is reminiscent of the large difference in effective Er size when it is doped in Si versus GaN hosts [4]. These results serve to confirm the predictions of low As solubility in GaN, and support understanding the very different behavior for rare-earth dopants.

[1] J. Neugebauer and C. G. Van de Walle, "Electronic structure and phase stability of GaAs_{1-x}N_x alloys", *Phys. Rev. B* **51**, 10568 (1995).

[2] C. G. Van de Walle and J. Neugebauer, "Arsenic Impurities in GaN", *Appl. Phys. Lett.* **76**, 1009 (2000).

[3] For example, see refs. in A. Bell, F. A. Ponce, S. V. Novikov, C. T. Foxon, and I. Harrison, "The Nature of Arsenic Incorporation in GaN", *Appl. Phys. Lett.* **79**, 3239 (2001).

[4] P. H. Citrin, P. A. Northrup, R. Birkhahn, and A. J. Steckl, "Local Structure and Bonding of Er in GaN: A Contrast with Er in Si", *Appl. Phys. Lett.* **76**, 2865 (2000).

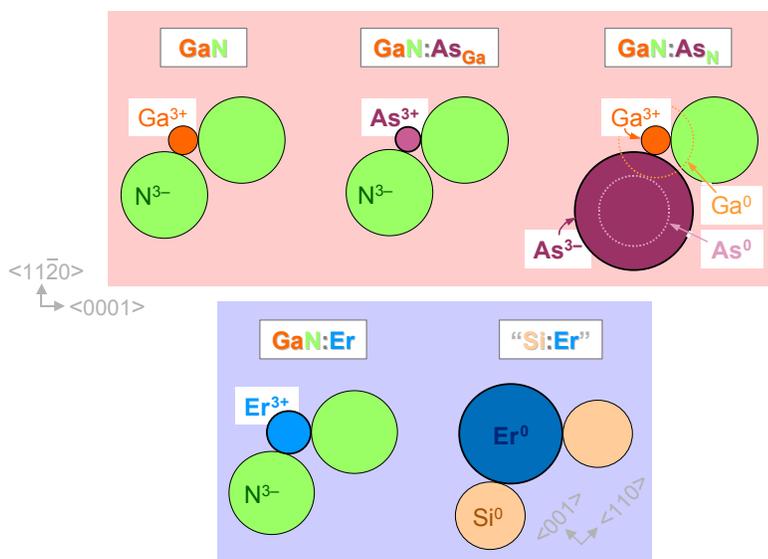


Fig. 1. Dopant atom charge-state/size as a function of lattice site and host.